# Knowledge-Based Thermodynamic Property Data Prediction System

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Thermodynamic property data play a vital role in scientific research and industries spanning chemistry and chemical engineering, pharmaceuticals, environmental protection, and food production. According to Chemical Abstract Service, there are currently more than 20 million registered and structurally elucidated compounds and over 5 million commercially available chemicals. However, only a small number of compounds have been experimentally studied. For example, while vapor-liquid critical properties are essential in corresponding-states modeling of equilibrium thermodynamic and transport property data, there are only around 700 substances with experimental critical data in existence. Consequently, this leads to a high demand for the development of predictive models of thermodynamic properties. In this respect, one of the most important problems is quality of the data predicted by models. The quality of predicted data is determined by many factors, such as, predictive ability of models, effect of uncertainty of the experimental data on model parameters, effect of number of the compounds on model parameters; impact of diversity and complexity of the data sets on generating parameters and on testing models, structure characteristics of the compound being predicted, uncertainty analysis of predicted values based on molecular similarity, theoretical foundation of the model, and applicability of the model under a given condition. In research and development of process design, the users of models not only require the best models, but also need to be given the information on how good the best models are. Sufficient knowledge of these factors is essential in providing high-quality information for predicted thermodynamic values. A knowledge-based computer system has been developed at NIST/TRC, aiming at automation of model evaluation and selection, and providing explanatory and analytical information and knowledge for the models of interest to users. This presentation will mainly introduce our effort in establishing a knowledge system and application in the prediction of thermodynamic property values of organic compounds, in combination with the NIST/TRC Source data system.